Textures and Microstructures, 1982, Vol. 5, pp. 87–94
0730–3300/82/0502–0087 $06.50/0

Reproducible Textures

H. J. BUNGE

Institut für Metallkunde und Metallphysik, Technische Universität, Clausthal-Zellerfeld—F.R.G.

and
C. ESLING

Laboratoire de Métallurgie Structurale, Université de Metz, Ile du Saulcy—57045 Metz Cedex—France

(Received January 5, 1982; in final form February 23, 1982)

Dedicated to Prof. G. Wassermann for his 80th birthday.

The orientation distribution function of a textured polycrystalline material may be split into an even and odd part; the latter is not reproducible from pole figure measurements as has been recently shown. The class of textures containing only a reproducible part is considered. In the case of axially symmetric textures (fibre textures), these take on a very simple form. They are, however, not the only type of reproducible textures as has been assumed. A sample having a reproducible texture is centrosymmetric, even in the most general case of non-centrosymmetric, enantiomorphic crystals of one crystal form only. Symmetry elements of this kind have been called non-conventional ones. They may be described by black-and-white or Shubnikov groups. Reproducible textures correspond to a non-conventional centre of inversion as an element of sample symmetry and vice versa.

The texture of a polycrystalline material is described completely by the orientation distribution function $f(g)$ of its crystallites. The orientation g may be specified by Euler angles $\varphi_1\Phi\varphi_2$. The function $f(g)$ is thus a function of three variables. In the specific case of fibre textures, the orientation distribution is independent of the angle φ_1. The texture problem is then reduced to a two dimensional one. The distribution function can be developed into a series of generalized spherical harmonics (Bunge, 1969; Bunge, 1982; Bunge and Esling, 1982)

$$f(g) = \sum_{l=0(1)}^{\infty} \sum_{m=-l}^{+l} \sum_{n=-l}^{+l} C_l^{mn} T_l^{mn}(g) \tag{1}$$

which may be split into the parts of even and odd values of the index l respectively (Matthies, 1979)

$$f(g) = \tilde{f}(g) + \tilde{\tilde{f}}(g) \tag{2}$$

In order for such a function to be a possible texture function it is necessary that it be nowhere negative.

$$f(g) \geqslant 0 \tag{3}$$

When the texture function $f(g)$ is given, the coefficients C_l^{mn} can be expressed by the integral

$$C_l^{mn} = (2l+1)\int f(g)\, T_l^{*mn}(g)\, dg \tag{4}$$

If the texture consists of a finite number of individual crystals having the orientations g_i and the volume fractions V_i then Eq. (4) can be transformed into

$$C_l^{mn} = (2l+1)\sum_i V_i T_l^{*mn}(g_i) \tag{5}$$

It has been shown by Matthies (1979 and 1980a, b, c, d) and by the authors (Muller *et al.*, 1981; Esling *et al.*, 1982) that the even part of the texture function $\tilde{f}(g)$ can be calculated (reproduced) from experimental pole figures. The odd part $\tilde{\tilde{f}}(g)$ is "invisible" in pole figures. It can only be concluded indirectly in certain favourable cases by turning the positivity condition of the ODF to advantage; this can be achieved in general terms by making use of Eq. (3) (Bunge and Esling, 1979a, b, Esling *et al.*, 1981a, b) or by means of more specific model functions (Lücke *et al.*, 1981). The even part $\tilde{f}(g)$ has thus been called the reproducible part of the texture function.

REPRODUCIBLE TEXTURES

A texture, the odd part of which is zero, can be completely reproduced from pole figure measurements. We will call it a reproducible texture $f_r(g)$. It is defined by

$$\tilde{\tilde{f}}_r(g) \equiv 0 \tag{6}$$

The reproducibility condition Eq. (6) is expressed in the coefficients C_l^{mn} by the condition

$$C_l^{mn} = 0 \qquad \text{for } l = \text{odd} \tag{7}$$

If the texture consisted of a finite number of crystallites the reproducibility condition would require an infinite number of conditions Eq. (7) to be fulfilled which is generally not possible with a finite number of variables g_i. Hence, a reproducible texture must always consist of an infinite number of crystallites i.e. the texture function must be a "true" distribution function in the statistical sense.

The even part of a given texture function $\tilde{f}(g)$ is generally not a reproducible texture because it may violate Eq. (3).

The most trivial reproducible texture is the random distribution

$$f(g) \equiv 1 \tag{8}$$

In its series expansion only the coefficient with $l = 0$ is different from zero.

A non-trivial class of reproducible textures has the form

$$f_r(g) = 1 + \frac{1}{a} T_{2l}^{mn}(g) \tag{9}$$

where a is larger than the absolute maximum negative value of the harmonic T_{2l}^{mn}. Two functions of this type have been given explicitly by Bunge and Esling (1979).

The most general reproducible texture can be written in the form

$$f_r(g) = 1 + \frac{1}{a} \sum_{l=2(2)}^{\infty} \sum_{m=-l}^{+l} \sum_{n=-l}^{+l} C_l^{mn} T_l^{mn}(g) \tag{10}$$

where a is larger than the absolute maximum negative value of the threefold sum. If the series is extended to infinity, then a finite value of a may not exist. But for any finite sum, it does exist. In Eq. (10) the threefold sum is the most general expression of an even function and the factor $1/a$ provides the necessary restrictions in the variation ranges of its coefficients C_l^{mn}/a in order not to violate Eq. (3).

COMPENSATORY TEXTURES

If $f(g)$ is a non-reproducible texture we may wonder whether it is always possible to make it reproducible by adding to it crystals with an appropriate orientation distribution function, i.e. by adding an appropriate texture which we may call a compensatory texture $f^c(g)$ to $f(g)$. If $f(g)$ is given by Eq. (2) then a compensatory texture may have the general form

$$f^c(g) = \tilde{f}'(g) - \frac{1}{\lambda} \cdot \tilde{\tilde{f}}(g), \quad \lambda > 0 \tag{11}$$

where $\tilde{f}'(g)$ is a certain even function which needs not necessarily obey Eq. (3). When the texture Eq. (11) is added to the texture Eq. (2) in an appropriate proportion, then the sum of the two textures is reproducible

$$f_r(g) = \frac{1}{1+\lambda}[f(g) + \lambda f^c(g)] \tag{12}$$

The factor $1/(1 + \lambda)$ is necessary in order for the resulting texture to be correctly normalized. According to Eq. (2) and (11) the odd part of Eq. (12) vanishes and if $f(g)$ and $f^c(g)$ obey Eq. (3), then the same is true for the function $f_r(g)$ Eq. (12). Hence, $f_r(g)$ is a reproducible texture and $f^c(g)$ is a compensatory texture.

If $f^c(g)$ is a texture compensatory to $f(g)$, then we can find a whole class of compensatory texture by adding $f^c(g)$ any reproducible texture $f_r(g)$ in any proportion γ:

$$f'^c(g) = \frac{1}{1+\gamma}[f^c(g) + \gamma f_r(g)] \tag{13}$$

One particular form of Eq. (11) is obtained when $\tilde{f}'(g)$ is the random distribution. In this case Eq. (11) takes on the form

$$f^c(g) = 1 - \frac{1}{a}\tilde{\tilde{f}}(g) \tag{14}$$

where a is larger than the maximum positive value of $\tilde{\tilde{f}}(g)$. The reproducible texture obtained from $f(g)$ by adding the compensatory texture Eq. (14) has the form

$$f_r(g) = \frac{1}{1+a}\tilde{f}(g) + \frac{a}{1+a} \tag{15}$$

Hence, a reproducible part of any texture can be made a reproducible texture itself if a sufficient amount of random texture is added. It is thus always possible to make any texture reproducible by adding further crystallites to it.

FIBRE TEXTURES

Fibre textures are independent to the Euler angle φ_1. They can be represented in form of a series expansion (Bunge, 1969; Bunge, 1982; Bunge and Esling, 1982).

$$f(h) = \sum_{l=0(1)}^{\infty} \sum_{m=-l}^{+l} C_l^m K_l^m(h) \tag{16}$$

where $K_l^m(h)$ are surface spherical harmonics and $h = \{\Phi\ \varphi_2\}$ represents the crystallographic direction parallel to the fibre axis. The positivity condition Eq. (3) must also be fulfilled.

The distribution function

$$f^c(h) = \sum_{l=0(1)}^{\infty} \sum_{m=-l}^{+l} (-1)^l \; C_l^m K_l^m(h) \tag{17}$$

has the same even part as the function $f(h)$ but the opposite odd part. It can be written in the form

$$f^c(h) = \sum_{l=0(1)}^{\infty} \sum_{m=-l}^{+l} C_l^{mn} K_l^m(-h) = f(-h) \tag{18}$$

which follows from the property of spherical harmonics

$$K_l^m(-h) = (-1)^l K_l^m(h) \tag{19}$$

If the function $f(h)$ is nowhere negative then the same is true for $f(-h)$ since $+h$ and $-h$ vary in the same range.

Hence $f^c(h) = f(-h)$ is a compensatory texture to the texture $f(h)$ according to Eq. (11) with $\lambda = 1$.

$$f^c(h) = f(-h) = \tilde{f}(h) - \tilde{\tilde{f}}(h) \tag{20}$$

The sum of the two textures is a reproducible texture

$$f_r(h) = \frac{1}{2}[f(h) + f^c(h)] = \frac{1}{2}[f(h) + f(-h)] = \tilde{f}(h) \tag{21}$$

This has been shown by Matthies (1980) and Mücklich *et al.* (1980) who have, however, averred that this was the only existing case of a reproducible texture except for the trivial one, Eq. (8).

According to Eq. (21) the reproducible part of any possible fibre texture is a possible reproducible texture itself.

Equation (20) is a particularly simple form of a compensatory texture and Eq. (21) is a particularly simple reproducible texture. Equation (21) may still be simplified if one assumes that the distributiom function $f(h)$ has the character of a δ-function i.e. if it is different from zero only in the orientation

$$h_o = \{\Phi^o, \varphi_2{}^o\} \tag{22}$$

The texture

$$f_r(h) = \frac{1}{2}[\delta(h_o) + \delta(-h_o)] \tag{23}$$

is a reproducible texture and it is composed of only two ideal "orientations" in the orientation space $\{\Phi, \varphi_2\}$. This seems to contradict the statement made in connection with Eq. (7) that a reproducible texture must consist of an infinite number of crystals. One has however to keep in mind that an ideal fibre texture Eq. (22) consists of an infinite number of crystals which are distinguished by the third Euler angle φ_1. Reproducible textures of the form Eq. (23) are thus but a very simple form of an infinite manifold of crystal orientations. Only in this respect are they exceptional with reference to the general case of reproducible textures.

NON-CONVENTIONAL SAMPLE SYMMETRY

So far, we have not yet taken crystal symmetry into account. The above considerations are therefore valid for the most general case, i.e. crystals without any kind of symmetry. Such crystals are enantiomorphic. They exist in a right-handed and a left-handed form. If both forms are present in the sample simultaneously then two texture functions corresponding to the right-handed and the left-handed fraction respectively must be specified (Esling *et al.*, 1980a, b; Esling, 1981). We may assume that $f(g)$, Eq. (1) represents one of them.

The axis distribution function $A(h,y)$ is defined by the integral of the orientation distribution function $f(g)$ over all those orientations for which the crystal direction h is parallel to the sample direction y

$$A(h,y) = \frac{1}{2\pi} \int_{h \| y} f(g)\, dg \tag{24}$$

It is expressed by the coefficients C_l^{mn}

$$A(h,y) = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \sum_{n=-l}^{+l} \frac{4\pi}{2l+1} C_l^{mn} K_l^{*m}(h) K_l^n(y) \tag{25}$$

where K_l^m are the surface spherical harmonics. For a reproducible texture, containing terms of even order only, it follows with Eq. (19)

$$A_r(h,y) = A_r(h,-y) \tag{26}$$

This means the distribution of crystal directions h falling into the sample direction $-y$ is the same as the one in the sample direction $+y$. The two sample directions are equivalent with respect to the texture. The texture thus exhibits a centre of inversion as an element of the *sample* symmetry. (Note that we have assumed that the crystal symmetry does not contain the centre of inversion).

According to Eq. (24), Eq. (26) represents an integral relation which is to be fulfilled by a reproducible texture function

$$\int_{h \| y} f_r(g)\, dg = \int_{h \| -y} f_r(g)\, dg \tag{27}$$

A relation of this type cannot be fulfilled by a one-to-one relationship between crystals in different orientations as in the case of conventional symmetry elements. Symmetry elements of this type in the sample symmetry have been called non-conventional symmetry elements (Bunge *et al.*, 1982).

When the sample symmetry contains a non-conventional centre of inversion then the texture function is reproducible and vice versa.

A *conventional* centre of inversion as an element of the sample symmetry is obtained when the sample contains an equal volume fraction of right-handed and left-handed crystals and the amount of right-handed crystals in an orientation g is equal to the amount of left-handed crystals in the centrosymmetric orientation. This is a one-to-one relationship. It can be realized by one right-handed and one left-handed crystal in centrosymmetric orientations. A centre of inversion of this conventional type should be carefully distinguished from the non-conventional one defined by Eq. (27).

If finally the crystals themselves are centrosymmetric (crystal symmetry), then they can be looked at as a right-handed and a left-handed part in the centrosymmetric orientation which is equivalent to the last mentioned case. In this case, the centre of inversion of the crystal symmetry induces automatically a conventional centre of inversion in the sample symmetry.

In order to distinguish conventional and non-conventional symmetry elements in the sample symmetry, black-and-white or Shubnikov groups are required instead of the common point symmetry groups (Bunge *et al.*, 1980; Bunge *et al.*, 1982).

The reproducibility condition Eq. (7) results from Friedels law which makes the crystal direction $+h$ indistinguishable of the direction $-h$ in a "normal" polycrystal diffraction experiment. If anomalous scattering is taken into account, then Friedels law may be violated (Bunge and Esling, 1981). It has been shown that in this case various symmetry elements of second kind in the crystal symmetry as well as in the sample symmetry may give rise to various other forms of the reproducibility (or determinability) condition (Bunge *et al.*, 1982; Bunge, 1981). However, the considerations above are still valid in an analogous sense which is such that the condition of reproducibility of a texture is equivalent to the presence of a non-conventional symmetry element in the sample symmetry.

Acknowledgements

The authors thank Mr. J. C. Lejosne for the revision of the English text.

References

Bunge, H. J. *Mathematische Methoden der Texturanalyse.* Akademie Verlag, Berlin (1969).
Bunge, H. J. *Texture Analysis in Material Science.* Butterworths publ., London, in print (1982).

Bunge, H. J. *Tecnhiques of Texture Analysis.* Proceedings of the Sixth International Conference on Textures. Tokyo (1981).
Bunge, H. J. and Esling, C. *Texture* **3**, 169 (1979).
Bunge, H. J. and Esling, C. *Journal de Physique Lettres* **40**, 627 (1979a).
Bunge, H. J. and Esling, C. *C.R. Acad. Sc. Paris* **B 289**, 163 (1979b).
Bunge, H. J. and Esling, C. *J. Appl. Cryst.* **14** (1981).
Bunge, H. J. and Esling, C. *Quantitative Texture Analysis.* D.G.M., Metallurgy Information, New-York, Oberursel (1982).
Bunge, H. J., Esling, C. and Muller, J. *J. Appl. Cryst.* **13**, 544 (1980).
Bunge, H. J., Esling, C. and Muller, J. *Acta Cryst.* in press (1982).
Esling, C., Bunge, H. J. and Muller, J. *Journal de Physique Lettres* **41**, 543 (1980a).
Esling, C., Bunge, H. J. and Muller, J. *C.R. Acad. Sc. Paris* **B 291**, 263 (1980b).
Esling, C., Bechler-Ferry, E. and Bunge, H. J. *J. Physique Lettres* **42**, 141 (1981a).
Esling, C., Bechler-Ferry, E. and Bunge, H. J. *C.R. Acad. Sc. Paris* **292**, 159 (1981b).
Esling, C. *Effets des symétries des cristaux, des échantillons et de la diffraction sur la définition et la détermination de la fonction de texture.* University of Metz, Thesis (1981).
Esling, C., Muller, J. and Bunge, H. J. *The determinability of the ODF by the inversion of pole figures.* In Quantitative Texture Analysis, D.G.M., Metallurgy Information, New-York, Oberursel, in press (1982).
Lücke, K., Pospiech, J., Virnich, K. H. and Jura, J. (1981). *Acta Metall.* **29**, 167–185.
Matthies, S. *Phys. Stat. Sol.* **B 92**, K135 (1979).
Matthies, S. *Kristall u. Technik* **15**, 431 (1980a).
Matthies, S. *Kristall u. Technik* **15**, 601 (1980b).
Matthies, S. *Kristall u. Technik* **15**, 823 (1980c).
Matthies, S. *Kristall u. Technik* **15**, 1189 (1980d).
Matthies, S. *Phys. Stat. Sol.* **(b) 98**, K113 (1980).
Mücklich, A., Matthies, S. and Hennig, K. *Z. Metallkunde* **71**, 777 (1980).
Muller, J., Esling, C. and Bunge, H. J. *Journal de Physique* **42**, 161 (1981).